

# On mathematical foundation of the Brownian motor theory.

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## Abstract

The paper contains mathematical justification of basic facts concerning the Brownian motor theory. The homogenization theorems are proved for the Brownian motion in periodic tubes with a constant drift. The study is based on an application of the Bloch decomposition. The effective drift and effective diffusivity are expressed in terms of the principal eigenvalue of the Bloch spectral problem on the cell of periodicity as well as in terms of the harmonic coordinate and the density of the invariant measure. We apply the formulas for the effective parameters to study the motion in periodic tubes with nearly separated dead zones.

**Keywords.** Brownian motors, diffusion, effective drift, effective diffusivity, Bloch decomposition.

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## 1 Introduction

The paper is devoted to mathematical theory of Brownian (molecular) motors. The concept of a Brownian motor has fundamental applications in the study of transport processes in living cells and (in a slightly different form) in the porous media theory. There are thousands of publications in the area of Brownian motors in the applied literature. For example, the review by P. Riemann [6] contains 729 references. Most of these publications are in physics or biology journals and are not mathematically rigorous. Some of them are based on numerical computations.

Consider a set of particles with an electrical charge performing Brownian motion in a tube  $\Omega$  with periodic (or stationary random) cross section (see Fig. 1).

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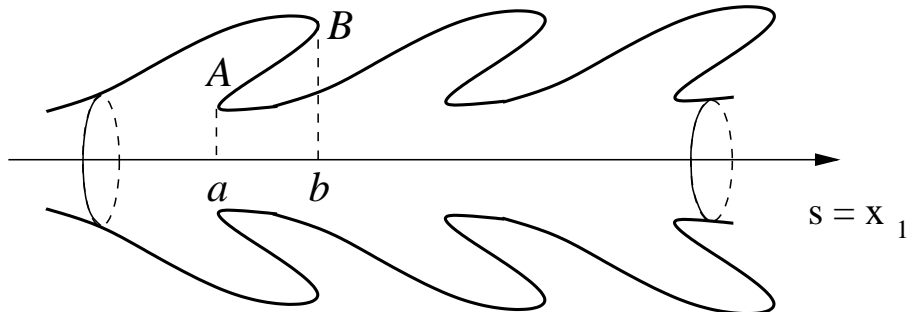


Figure 1: A periodic tube  $\Omega$  with “fingers”. One can expect that  $V_{\text{eff}} < |V_{\text{eff}}^-|$ .

We will assume that the axis of  $\Omega$  is directed along the  $x_1$ -axis. Let's apply a constant external electric field  $E$  along the axis of  $\Omega$ . Then the motion of the particles consists of the diffusion and the Stocks drift, and the corresponding generator has the form

$$Lu = \Delta u + V \frac{\partial u}{\partial x_1}, \quad V = V(E),$$

complemented by the Neumann boundary condition on  $\partial\Omega$  (we assume the normal reflection at the boundary).

One can expect that the displacement of the particles on the large time scale may be approximated (due to homogenization) by a one-dimensional diffusion process  $\bar{x}_1(t)$  along the  $x_1$ -axis with an effective drift  $V_{\text{eff}}$  and an effective diffusivity  $\sigma^2$ , which depend on  $V$  and the geometry of the tube  $\Omega$ . If we reverse the direction of the external field from  $E$  to  $-E$ , then the corresponding effective drift  $V_{\text{eff}}^-$  and the corresponding effective diffusivity  $(\sigma^-)^2$  will be, generally, different from  $V_{\text{eff}}$  and  $\sigma^2$  when  $\Omega$  is not symmetric with respect to the reflection  $x_1 \rightarrow -x_1$ . For example, one can expect that  $V_{\text{eff}} < |V_{\text{eff}}^-|$  for  $\Omega$  shown in Fig. 1. The difference between the effective parameters can be significant. Then by changing the direction of the exterior electric field  $E$  periodically in time, one could construct a constant drift in, say, the negative direction of  $x_1$  and create a device (motor) producing energy from Brownian motion.

The idea of molecular motors goes back to M. Smoluchowski, R. Feynman, L. Brillouin. Starting from the 1990-s, it became a hot topic in chemical physics, molecular biology, and thermodynamics. The following natural problem must be solved by mathematicians:

1. The homogenization procedure (reduction to a one-dimensional problem) must be justified.
2. Expressions for effective parameters  $V_{\text{eff}}, \sigma^2$  in terms of an appropriate PDE or a spectral problem on the period of  $\Omega$  (in the case of periodic tubes) must be found.
3. For some natural geometries of  $\Omega$  that include a small parameter, asymptotic expressions for effective parameters need to be obtained.

We solve the first two problems here using an analytic approach that justifies the homogenization procedure and allows us to express the effective parameters in terms of

the principal eigenvalue of a spectral problem on one period of  $\Omega$ . We will also provide a couple of simple consequences of the obtained formulas. We show that  $dV_{\text{eff}}/dV = \sigma^2 > 0$  when  $V = 0$ . Thus, since  $V_{\text{eff}}$  is analytic in  $V$ , it is a strictly monotone function of  $V$  when  $|V|$  is small enough. Simple asymptotic formulas for the effective parameters will be justified for periodic tubes with nearly separated dead zones. Note that the first two problems listed above also can be solved with probabilistic techniques similar to those used for homogenization of periodic operators in  $\mathbb{R}^d$ , as we'll discuss in a forthcoming paper.

Our approach is based on the Bloch decomposition. Recently several papers appeared (see [2, 3] and references there), where the Bloch decomposition was used to study homogenization problems in periodic media. It was shown that this approach has many advantages (when it is applicable). So far, this approach was applied to self-adjoint elliptic equations in the whole space or in a domain with a finite boundary. The symmetry and the existence of a bounded inverse operator were essential there.

We consider a parabolic problem. It is non-self-adjoint due to the drift, which can not be neglected since it is essential for applications. Besides, the homogenization is applied only with respect to one variable. All these features (the non-symmetry is the main difficulty) make the problem under consideration essentially different from the applications of the Bloch decomposition in the homogenization mentioned above.

We also would like to note the presence of the boundary integral term in the formula for the effective drift (see Theorem 2.5). In probabilistic terms, it arises from the re-normalized time spent by the Brownian motion with the drift on the boundary (local time). Our next paper based on a probabilistic approach to the problem will contain the detailed analysis of the asymptotic behavior of the effective parameters with respect to the parameters describing the geometry of the domain.

The plan of the paper is as follows. Lemma 2.2 describes the properties of the principal eigenvalue  $\lambda_0 = \lambda_0(\theta)$  of the Bloch spectral problem on the cell of periodicity of  $\Omega$ . The main results on homogenization are obtained in Theorems 2.1 and 2.3. In particular, it is shown there that the effective drift  $V_{\text{eff}}$  and the effective diffusivity  $\sigma^2$  are given by the coefficients of the Taylor expansion of the eigenvalue  $\lambda_0(\theta)$ . To be more exact,  $\lambda_0(\theta) = iV_{\text{eff}}\theta - \sigma^2\theta^2 + O|\theta|^3$ ,  $\theta \rightarrow 0$ . Expressions for the effective parameters through the harmonic coordinate and the invariant measure are given in Theorem 2.5. The latter formulas are applied to a particular class of domains in the last section. Periodic tubes with nearly separated dead zones are considered there. We rigorously justified the asymptotic formula for the effective diffusivity, which was found earlier for domains with somewhat simpler geometry in [1], [4].

## 2 Description of the model and main results.

Consider a tube  $\Omega \subset \mathbb{R}^d$ ,  $d \geq 2$ , periodic in  $x_1$  with period 1, with a smooth boundary  $\partial\Omega$  (see Fig. 1). Denote by  $S_{x_1}$  the cross-section of  $\Omega$  by the plane  $\mathbb{R}^{d-1}$  orthogonal to the

$x_1$ -axis at the point  $x_1$ . We assume that  $S_{x_1}$  is bounded (and periodic with respect to  $x_1$ ).

In the simplest case, the boundary of the cross-section is a function of the angular variables. For instance,  $S_{x_1}$  is the ball of the radius  $R(x_1)$  if  $\partial\Omega$  is the surface of revolution. However, in general it may have a very complicated form. For example,  $\Omega$  in Fig.1 contains “fingers” (“dead ends” in the terminology of [7], [8]), and  $S_{x_1}$  is not connected when  $a < x_1 < b$ .

Consider the cell of periodicity in  $\Omega$  defined as  $\Omega' = \Omega \cap \{0 < x_1 < 1\}$ . It is assumed that the compact manifold obtained from  $\Omega'$  by gluing  $S_0$  to  $S_1$  is connected. For transparency, one can assume that  $\Omega'$  itself is connected. For example,  $\Omega'$  in Fig.1 is connected if the origin is slightly to the left of  $a$ . It is not connected if the origin is the midpoint between  $a$  and  $b$ , however, it still forms a connected manifold after gluing  $S_0$  to  $S_1$ . One also can define a connected cell of periodicity  $\Omega'$  in Fig.1 using planes  $\mathbb{R}^{d-1}$  through  $(a+b)/2$  and  $(a+b)/2+1$  by cutting only the central narrow part of  $\Omega$ , but not cutting the fingers. In the latter case, we use the notation  $S_0, S_1$  not for the whole cross-sections of  $\Omega$ , but for the parts of the boundary of  $\Omega'$  that belong to the corresponding  $\mathbb{R}^{d-1}$  planes.

Denote the exterior normal to  $\partial\Omega$  by  $n$ . Let  $x = (s, z)$ , where  $s = x_1$ ,  $z = (x_2, \dots, x_d)$ . Consider the following parabolic problem in the tube  $\Omega$ :

$$\frac{\partial u}{\partial t} = \Delta u + V \frac{\partial u}{\partial s}, \quad x \in \Omega; \quad \frac{\partial u}{\partial n}|_{\partial\Omega} = 0; \quad u(0, x) = \varphi(\varepsilon s, z), \quad x \in \Omega, \quad (1)$$

where  $\varphi \in L_{1,\text{com}}(\mathbb{R}^d)$  (the space of integrable functions with compact supports).

The main results of the first part of the paper are stated in the following two theorems. Theorem 2.1 specifies the asymptotic behavior, as  $\varepsilon \downarrow 0$ , of the solution  $u$  of the problem (1) in terms of the solution  $w$  of the one-dimensional problem

$$\frac{\partial w}{\partial t} = \sigma^2 \frac{\partial^2 w}{\partial s^2} + V_{\text{eff}} \frac{\partial w}{\partial s}, \quad s \in \mathbb{R}; \quad w|_{t=0} = w_0(s, \varepsilon s). \quad (2)$$

Here  $\sigma^2$  is the effective diffusivity,  $V_{\text{eff}}$  is the effective drift, and the initial function  $w_0(s, \varepsilon s)$  **Remove the arguments?** is an average of  $\varphi$  in  $z$ -variable and will be defined later in (5). This theorem provides also the main term of asymptotics of  $u$  in terms of the solution  $\bar{w}$  of a one-dimensional,  $\varepsilon$ -independent problem if  $\varphi$  is smooth. The second theorem describes the effective parameters  $\sigma^2$  and  $V_{\text{eff}}$  in terms of the problem on the cell  $\Omega'$ .

We will use notation  $O(\varepsilon)$  for functions  $f$  such that  $|f| < C\varepsilon$ ,  $\varepsilon \downarrow 0$ .

**Theorem 2.1.** 1) Let  $\varphi \in L_{1,\text{com}}(\mathbb{R}^d)$ . Then for each  $t_0 > 0$ ,

$$u = w + O(\varepsilon), \quad t > \frac{t_0}{\varepsilon^2},$$

where  $w$  is the solution of (2) and  $w_0$  is defined in (5).

2) Let  $\varphi$  and its derivative  $\varphi_s$  be continuous bounded functions with compact supports. Let  $t = \frac{\tau}{\varepsilon^2}$ ,  $s = \frac{s - V_{\text{eff}}\tau}{\varepsilon}$  and let  $\bar{u}(\tau, \varsigma, z) = u(t, s, z)$  be the function  $u$  written in the new variables. Then for each  $\tau_0 > 0$ ,

$$\bar{u} = \bar{w} + O(\varepsilon), \quad \tau > \tau_0,$$

where  $\bar{w}$  is the solution of the following  $\varepsilon$ -independent problem

$$\frac{\partial \bar{w}}{\partial \tau} = \sigma^2 \frac{\partial^2 \bar{w}}{\partial \varsigma^2}, \quad \varsigma \in \mathbb{R}; \quad \bar{w}|_{t=0} = \bar{\varphi}(\varsigma) = \int_0^1 w_0(s, \varsigma) ds,$$

**Remarks.** 1. An explicit form of  $\bar{\varphi}$  is given below in (5).

2. The proof of the theorem allows one to obtain explicit estimates of the reminder terms in the formulas above through the corresponding norms of  $\varphi$ .

We need to state one important lemma before we can formulate the second theorem. Denote by  $S^l$  the lateral part of the boundary  $\partial\Omega'$  of  $\Omega'$ , i.e.,  $S^l = \partial\Omega' \setminus [S_0 \cup S_1]$ . Consider the following eigenvalue problem on the cell  $\Omega'$ :

$$\Delta v + V \frac{\partial v}{\partial s} = \lambda v, \quad x \in \Omega'; \quad \frac{\partial v}{\partial n}|_{S^l} = 0; \quad v|_{S_1} = e^{i\theta} v|_{S_0}, \quad v'_s|_{S_1} = e^{i\theta} v'_s|_{S_0}. \quad (3)$$

This is an elliptic problem in a bounded domain, and for each  $\theta$  the spectrum of this problem consists of a discrete set of eigenvalues  $\lambda = \lambda_j(\theta)$ ,  $j \geq 0$ , of finite multiplicity.

**Lemma 2.2.** *Let  $\theta \in [-\pi, \pi]$ . There exists a simple eigenvalue  $\lambda = \lambda_0(\theta)$  of problem (3) in a neighborhood  $|\theta| < \delta$  of the origin  $\theta = 0$  and real constants  $V_{\text{eff}}, \sigma$  such that*

- 1)  $\lambda_0 = iV_{\text{eff}}\theta - \sigma^2\theta^2 + O(\theta^3)$ ,  $\theta \rightarrow 0$ , where  $\sigma^2 > 0$ ,
- 2)  $\text{Re}\lambda_0(\theta) < 0$ ,  $0 < |\theta| \leq \delta$ ,
- 3)  $\text{Re}\lambda_j(\theta) < -\gamma_1$ ,  $|\theta| \leq \delta$ ,  $j > 0$ ,  $\gamma_1 = \gamma_1(\delta) > 0$ ,
- 4)  $\text{Re}\lambda_j(\theta) < -\gamma_2$ ,  $\delta \leq |\theta| < \pi$ ,  $j \geq 0$ ,  $\gamma_2 = \gamma_2(\delta) > 0$ .

**Theorem 2.3.** *The effective diffusivity  $\sigma^2$  and effective drift  $V_{\text{eff}}$  defined in (2) coincide with the constants introduced in Lemma 2.2.*

Let us describe the averaged initial function  $\bar{\varphi}$ . We need the problem adjoint to problem (3). This problem has the form:

$$\Delta v - V \frac{\partial v}{\partial s} = \lambda v, \quad x \in \Omega'; \quad \left(\frac{\partial}{\partial n} - Vn_1\right)v|_{S^l} = 0; \quad v|_{S_1} = e^{i\theta} v|_{S_0}, \quad v'_s|_{S_1} = e^{i\theta} v'_s|_{S_0}, \quad (4)$$

where  $n_1 = n_1(x)$  is the first component of the normal vector  $n$ . Then  $\lambda = \bar{\lambda}_0(\theta)$  is an eigenvalue of problem (4). Let  $v = \psi_0^*(\theta, x)$  be the corresponding eigenfunction, and let  $\pi(x) = \psi_0^*(0, x)$  be the eigenfunction of (4) when  $\theta = 0$  (and  $\lambda_0 = \lambda_0(0) = 0$ ). Then  $w_0, \bar{\varphi}$  are defined as follows:

$$w_0(s, \varepsilon s) = \int_{S_s} \pi(s, z) \varphi(\varepsilon s, z) dz, \quad \bar{\varphi} = \int_0^1 \int_{S_s} \pi(s, z) \varphi(\varsigma, z) dz ds, \quad (5)$$

where  $S_a$  is the cross-section of  $\Omega$  by the plane through  $s = a$ .

The following lemma will be needed in order to prove the theorems above. Consider the non-homogeneous problem (3) in the Sobolev space  $H^2(S)$ :

$$(\Delta + V \frac{\partial}{\partial s} - \lambda)v = f, \quad x \in \Omega'; \quad \frac{\partial v}{\partial n}|_{S'} = 0; \quad v|_{S_1} = e^{i\theta}v|_{S_0}, \quad v'_s|_{S_1} = e^{i\theta}v'_s|_{S_0}. \quad (6)$$

This is an elliptic problem, and the resolvent

$$R_\lambda^\theta = (\Delta + V \frac{\partial}{\partial s} - \lambda)^{-1} : L_2(\Omega') \rightarrow H^2(\Omega')$$

is a meromorphic in  $\lambda$  operator with poles at a discrete set of eigenvalues  $\lambda = \lambda_j(\theta)$ . Denote by  $Q_\alpha$  the sector in the complex  $\lambda$ -plane that does not contain the negative semi-axis and is defined by inequalities  $-\pi + \alpha \leq \arg \lambda \leq \pi - \alpha$ .

**Lemma 2.4.** *For every  $\alpha > 0$  there exist constants  $R = R(\alpha)$  and  $C = C(\alpha)$  such that the region  $Q_{\alpha,R} = Q_\alpha \cap \{|\lambda| > R\}$  does not contain eigenvalues  $\lambda_j(\theta)$ , and the following estimate is valid for the solution  $v = R_\lambda^\theta f$  of the problem (6):*

$$|\lambda| \|v\|_{L_2(\Omega')} \leq C(\alpha) \|f\|_{L_2(\Omega')}, \quad \lambda \in Q_{\alpha,R}. \quad (7)$$

**Proof.** This lemma can be proved by referencing the standard a priori estimates for parameter-elliptic problems [5]. We will provide an independent proof. We multiply equation (6) by  $\bar{v}$  and integrate over  $\Omega'$ . This leads to

$$- \int_{\Omega'} (|\nabla v|^2 + \lambda |v|^2) dx + \int_{\Omega'} V v'_s \bar{v} dx = \int_{\Omega'} f \bar{v} dx. \quad (8)$$

The terms on the left in (8) can be estimated as follows

$$| \int_{\Omega'} (|\nabla v|^2 + \lambda |v|^2) dx | \geq c_1(\alpha) (\|\nabla v\|_{L_2(\Omega')}^2 + |\lambda| \|v\|_{L_2(\Omega')}^2), \quad \lambda \in Q_\alpha,$$

and

$$| \int_{\Omega'} V v'_s \bar{v} dx | \leq \frac{c_1(\alpha)}{2} \|v'_s\|_{L_2(\Omega')}^2 + \frac{V^2}{2c_1(\alpha)} \|v\|_{L_2(\Omega')}^2.$$

We put  $R = \frac{V^2}{[c_1(\alpha)]^2}$ . Then the absolute value of the left-hand side in (8) is estimated from below by  $\frac{c_1(\alpha)}{2} (\|\nabla v\|_{L_2(\Omega')}^2 + |\lambda| \|v\|_{L_2(\Omega')}^2)$  when  $\lambda \in Q_{\alpha,R}$ , and (8) implies that

$$\frac{c_1(\alpha)}{2} (\|\nabla v\|_{L_2(\Omega')}^2 + |\lambda| \|v\|_{L_2(\Omega')}^2) \leq \|f\|_{L_2(\Omega')} \|v\|_{L_2(\Omega')}, \quad \lambda \in Q_{\alpha,R}. \quad (9)$$

We omit the first term on the left and obtain (7).  $\square$

**Proof of Lemma 2.2.** Denote by  $H_\theta = \Delta + V \frac{\partial}{\partial s}$  the operator in  $L_2(\Omega')$  defined on the functions from the Sobolev space  $H^2(\Omega')$  satisfying the boundary conditions (3). One can

define the parabolic semi-group  $e^{tH_\theta}$ . Its integral kernel is the fundamental solution of the corresponding parabolic boundary value problem in  $\Omega'$ . When  $\theta = 0$ , this kernel is real and positive. Thus Perron-Frobenius theorem is applicable to the operator  $e^{tH_0}$ , i.e., the operator  $e^{tH_0}$  has a unique maximal eigenvalue  $\mu$  such that  $\mu > 0$ ,  $\mu$  is simple, the corresponding eigenfunction is positive, all the other eigenvalues  $\mu_j$  (perhaps complex) are strictly less than  $\mu$  in absolute value ( $|\mu_j| < \mu$ ), and the operator does not have strictly positive eigenfunctions with eigenvalues different from  $\mu$ .

We note that  $v_0 \equiv 1$  is an eigenfunction of  $H_0$  with the eigenvalue  $\lambda_0 = 0$ . Thus  $v_0$  is an eigenfunction of  $e^{tH_0}$  with the eigenvalue  $\mu = 1$ . Since  $v_0 > 0$ , from the Perron-Frobenius theorem it follows that  $\mu = 1$  is the maximal eigenvalue of  $e^{tH_0}$ . This implies that  $\text{Re}\lambda_j < \lambda_0 = 0$  for all the eigenvalues  $\lambda_j \neq 0$  of the operator  $H_0$ . Since the eigenvalues  $\lambda_j$  form a discrete set, from Lemma 2.4 it follows that there exists a  $\gamma > 0$  such that  $\text{Re}\lambda_j < -\gamma$  for all  $\lambda_j \neq 0$ .

Since  $H_\theta$  depends analytically on  $\theta$ , the location of the eigenvalues  $\lambda_j$  when  $\theta = 0$  and Lemma 2.4 imply that there exists  $\delta > 0$  such that the operator  $H_\theta$  has the following structure of the spectrum when  $|\theta| \leq \delta$ : the operator has a simple, analytic in  $\theta$  eigenvalue  $\lambda = \lambda_0(\theta)$ ,  $\lambda_0(0) = 0$ , and  $\text{Re}\lambda_j(\theta) < -\gamma_1 = -\gamma/2$  for all other eigenvalues  $\lambda_j(\theta)$  of  $H_\theta$ . The statement 3 of Lemma 2.2 is proved. Consider now the eigenvalue  $\lambda = \lambda_0(\theta)$  for purely imaginary  $\theta = iz$ ,  $z > 0$ . If  $v$  belongs to the domain of the operator  $H_{iz}$ , then  $\bar{v}$  also belongs to the domain of the operator  $H_{iz}$ . From here it follows that both  $\lambda = \lambda_0(iz)$  and  $\lambda = \overline{\lambda_0(iz)}$  are eigenvalues of  $H_{iz}$ . Since,  $\lambda = \lambda_0(\theta)$  is the unique eigenvalue in a neighborhood of the point  $\lambda = 0$ , it follows that  $\lambda_0(iz)$  is real. This implies statement 1 of Lemma 2.2, except the inequality  $\sigma^2 > 0$ . The latter inequality will be proved below (in Theorem 2.5) by a direct calculation of  $\sigma^2$  (see formula (26)). Thus it remains to justify statements 2 and 4. This will be done if we prove that for every  $\delta_1 > 0$ , there exists  $\gamma = \gamma(\delta_1) > 0$  such that  $\text{Re}\lambda_j(\theta) < -\gamma$  for all the eigenvalues of the operator  $H_\theta$  when  $\theta$  is real,  $\delta_1 \leq |\theta| \leq \pi$ .

Let us prove the latter estimate for the eigenvalues  $\lambda_j(\theta)$ ,  $\delta_1 \leq |\theta| \leq \pi$ . We fix an arbitrary rational  $\theta = \theta' = \frac{\pm m}{n}$  in the set  $\delta_1 \leq |\theta| \leq \pi$ . Consider the domain  $\widehat{\Omega} = \Omega \cap \{0 < x_1 < n\}$ , which consists of  $n$  elementary cells of periodicity  $\Omega^{(j)} = \Omega \cap \{j < x_1 < j+1\}$ ,  $0 \leq j \leq n-1$  ( $\Omega^{(0)}$  coincides with the previously introduced cell  $\Omega'$ ). The lateral side of the boundary of the domain  $\widehat{\Omega}$  will be denoted by  $\widehat{S}^l$ , and the parts of the boundary located in the planes through the points  $x_1 = 0$  and  $x_1 = n$  will be denoted by  $S_0$  and  $S_n$ , respectively. Let  $H_\theta^{(n)} = \Delta + V \frac{\partial}{\partial s}$  be the operator in  $L_2(\widehat{\Omega})$  that corresponds to the following analogue of the problem (3):

$$\Delta v + V \frac{\partial v}{\partial s} = \alpha v, \quad x \in \widehat{\Omega}; \quad \frac{\partial v}{\partial n} \Big|_{\widehat{S}^l} = 0; \quad v|_{S_n} = e^{in\theta} v|_{S_0}, \quad v'_s|_{S_n} = e^{in\theta} v'_s|_{S_0}. \quad (10)$$

We denote its eigenvalues by  $\alpha = \alpha_j$ , and we keep the notation  $\lambda = \lambda_j$  for the eigenvalues of this operator when  $n = 1$  (and  $\widehat{\Omega} = \Omega'$ ).

When  $\theta = \theta'$ , the conditions on  $S_0, S_n$  become the periodicity condition. Thus the spectrum of  $H_{\theta'}^{(n)}$  has the same structure as the spectrum of  $H_0$ , i.e.,  $\alpha_0 = 0$  is an eigenvalue



with the eigenfunction  $v_0 = 1$ , and

$$\operatorname{Re} \alpha_j < -\gamma < 0 \quad (11)$$

for all other eigenvalues  $\alpha_j$  of  $H_{\theta'}^{(n)}$ .

We compare the set  $\{\lambda_j\}$  of the eigenvalues of the operator  $H_{\theta'}$  and the set  $\{\alpha_j\}$  of the eigenvalues of the operator  $H_{\theta'}^{(n)}$ . The following inclusion holds:  $\{\lambda_j\} \subset \{\alpha_j\}$ . Indeed, if  $v$  is an eigenfunction of the operator  $H_{\theta'}$ , then one can construct the corresponding eigenfunction of  $H_{\theta'}^{(n)}$  with the same eigenvalue by defining it as  $e^{ij\theta}v$  in each elementary cell  $\Omega^{(j)} \subset \widehat{\Omega}$ ,  $0 \leq j \leq n-1$ . However, these two sets of eigenvalues do not coincide. In particular,  $\lambda = 0$  is not an eigenvalue of  $H_{\theta'}$  (while  $\alpha = 0$  is an eigenvalue of  $H_{\theta'}^{(n)}$ ). Indeed, from the simplicity of the eigenvalue  $\alpha = 0$  it follows that  $\lambda = 0$  could be an eigenvalue of  $H_{\theta'}$  only if  $v_0 = 1$  is its eigenfunction, but  $v_0$  does not satisfy the boundary conditions (3). Thus, (11) implies that  $\operatorname{Re} \lambda_j < -\gamma < 0$  for the set of eigenvalues of the operator  $H_{\theta'}$ . Then the same estimate with  $\gamma/2$  instead of  $\gamma$  is valid for the eigenvalues of  $H_{\theta}$  when  $\theta$  is in a small enough neighborhood of  $\theta' = \frac{\pm m}{n}$ . One can find a finite covering of the set  $\{\theta : \delta_1 \leq |\theta| \leq \pi\}$  by some of these neighborhoods. Thus, the desirable estimate of eigenvalues  $\lambda_j(\theta)$  is valid for all  $\theta$  of the set  $\{\theta : \delta_1 \leq |\theta| \leq \pi\}$ .  $\square$

**Proof of Theorems 2.1 and 2.3.** The solution  $u$  of problem (1) can be found using the Laplace transform in  $t$ :

$$u = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} v(\lambda, x) e^{\lambda t} d\lambda, \quad a > 0,$$

where  $v \in L_2(\Omega)$  is the solution of the corresponding stationary problem:

$$\Delta v + V \frac{\partial v}{\partial s} - \lambda v = -\varphi, \quad x \in \Omega; \quad \frac{\partial v}{\partial n} \Big|_{\partial\Omega} = 0. \quad (12)$$

In order to solve (12), we apply the Bloch transform in the variable  $s = x_1$ :

$$w(x) \rightarrow \widehat{w}(\theta, x) = \sum_{-\infty}^{\infty} w(s - n, z) e^{in\theta}, \quad \theta \in (-\pi, \pi), \quad x \in \Omega.$$

This map is unitary (up to the factor  $1/\sqrt{2\pi}$ ) from  $L_2(\Omega)$  to  $L_2([-\pi, \pi]) \times L_2(\Omega')$ , and the inverse transform is given by

$$w(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \widehat{w}(\theta, x) d\theta, \quad x \in \Omega.$$

Note that function  $e^{-i\theta s} \widehat{w}(\theta, x)$  is periodic in  $s$ . Thus the knowledge of  $\widehat{w}$  on  $\Omega'$  allows one to recover  $\widehat{w}$  on the whole tube  $\Omega$ .



The Bloch transform reduces problem (12) to a problem for  $\widehat{v}$  on the cell of periodicity  $\Omega'$ . The latter problem has form (6) with  $f = -\widehat{\varphi}$ , i.e.,  $\widehat{v} = -R_\lambda^\theta \widehat{\varphi}$ . Thus

$$u(t, x) = \frac{-1}{4\pi^2 i} \int_{a-i\infty}^{a+i\infty} \int_{-\pi}^{\pi} R_\lambda^\theta \widehat{\varphi} e^{\lambda t} d\theta d\lambda, \quad x \in \Omega. \quad (13)$$

Function  $R_\lambda^\theta \widehat{\varphi}$  here is defined in  $\Omega'$ , but it is extended to the whole tube  $\Omega$  in such a way that  $e^{-i\theta s} R_\lambda^\theta \widehat{\varphi}$  is periodic in  $s$ .

Now that formula (13) for  $u$  is established, we are going to study the asymptotic behavior of  $u$  as  $\varepsilon \rightarrow 0$ . We split  $u$  as  $u = u_1 + u_2$ , where the terms  $u_1, u_2$  are given by (13) with integration in  $\theta$  over sets  $|\theta| \leq \delta$  and  $\delta \leq |\theta| \leq \pi$ , respectively. We choose  $\delta$  small enough, so that Lemma 2.2 holds, and then make it even smaller (if needed) to guarantee that  $-\frac{\gamma_1}{2} < \operatorname{Re} \lambda_0(\theta) \leq 0$ ,  $|\theta| \leq \delta$ .

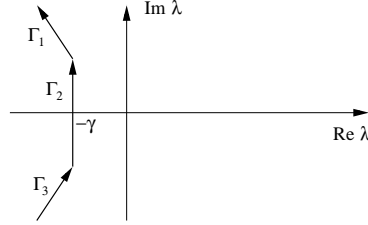


Figure 2: Contour  $\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_3$ , where  $\gamma$  coincides with  $\gamma_1$  or  $\gamma_2$  defined in Lemma 2.2, and  $\Gamma_2$  is long enough, so that the estimate (7) is valid on  $\Gamma_1$  and  $\Gamma_3$ .

Let us show that  $u_2$  does not contribute to the main term of asymptotics of  $u$ . Lemmas 2.4 and 2.2 allow us to rewrite  $u_2$  in the form

$$u_2(t, x) = \frac{-1}{4\pi^2 i} \int_{\Gamma} \int_{\delta < |\theta| < \pi} R_\lambda^\theta \widehat{\varphi} e^{\lambda t} d\theta d\lambda, \quad x \in \Omega, \quad (14)$$

where  $\Gamma$  is the contour shown in Fig. 2 with  $\gamma = \gamma_2$ . From Lemmas 2.4 and 2.2 it follows that

$$\|R_\lambda^\theta \widehat{\varphi}\|_{L_2(\Omega')} \leq \frac{c_1}{1 + |\lambda|} \|\widehat{\varphi}\|_{L_2(\Omega')}, \quad \lambda \in \Gamma, \quad \delta < |\theta| < \pi.$$

Thus

$$\begin{aligned} \int_{\delta < |\theta| < \pi} \|R_\lambda^\theta \widehat{\varphi}\|_{L_2(\Omega')} d\theta &\leq \frac{c_1}{1 + |\lambda|} \|\widehat{\varphi}\|_{L_2(\Omega') \times L_2(|\theta| < \pi)} = \frac{c_2}{1 + |\lambda|} \|\varphi(\varepsilon s, z)\|_{L_2(\Omega)} \\ &\leq \frac{c_2}{(1 + |\lambda|)\sqrt{\varepsilon}} \|\varphi(x)\|_{L_2(\mathbb{R}^d)}, \quad \lambda \in \Gamma. \end{aligned} \quad (15)$$

One can replace  $\Omega'$  here by a shifted cell of periodicity  $\Omega^{(j)}$  defined by inequalities  $j < x_1 < j + 1$ , since the function  $e^{-i\theta x_1} R_\lambda^\theta \widehat{\varphi}$  is periodic in  $x_1$ . We put (15) with  $\Omega'$  replaced by  $\Omega^{(j)}$  into (14) and estimate the integral over  $\Gamma$ . This gives

$$\|u_2(t, x)\|_{L_2(\Omega^{(j)})} \leq \frac{c}{\sqrt{\varepsilon}} e^{-\gamma t} \|\varphi(x)\|_{L_2(\mathbb{R}^d)},$$

where  $c$  does not depend on  $j$ .

Now one can obtain a uniform estimate of  $u_2$  by using the following inequality for the Green function  $G(t, x, y)$  of the problem (1):  $|G(1, x, y)| < ae^{-b(x_1-y_1)^2}$ , which implies that

$$\begin{aligned} |u_2(t, x)| &\leq \int_{\Omega} |G(1, x, y)u_2(t-1, y)|dy \leq \frac{A}{\sqrt{\varepsilon}} e^{-\gamma t} \sum_{j=-\infty}^{\infty} e^{-b(x_1-j)^2} \|\varphi(x)\|_{L_2(\mathbb{R}^d)} \\ &\leq \frac{C}{\sqrt{\varepsilon}} e^{-\gamma t} \|\varphi(x)\|_{L_2(\mathbb{R}^d)}, \quad x \in \Omega, \quad t > 1. \end{aligned}$$

In particular,  $u_2 = O(\varepsilon)$  when  $t > t_0/\varepsilon^2$ . Hence  $u_2$  does not contribute to the main term of the asymptotics of  $u$ .

In order to study  $u_1$ , we also shift the contour of integration (in  $\lambda$ ) to  $\Gamma$ . Now we take  $\gamma = \gamma_1$ , and in this case the simple pole of  $R_{\lambda}^{\theta}$  at  $\lambda = \lambda_0(\theta)$  must be taken into account. The residue at this pole of the integral kernel of the operator  $R_{\lambda}^{\theta}$  is equal to  $-\psi(\theta, x)\overline{\psi^*}(\theta, y)$ , where  $\psi$  is the eigenfunction of the problem (3) and  $\psi^*$  is the eigenfunction of the problem (4) (the residue is a negative operator). Thus

$$u_1(t, x) = \frac{1}{2\pi} \int_{|\theta| < \delta} \int_{\Omega'} \psi(\theta, x) \overline{\psi^*}(\theta, y) e^{\lambda_0(\theta)t} \widehat{\varphi} dy d\theta - \frac{1}{4\pi^2 i} \int_{\Gamma} \int_{|\theta| < \delta} R_{\lambda}^{\theta} \widehat{\varphi} e^{\lambda t} d\lambda, \quad x \in \Omega, \quad (16)$$

where the functions  $\psi, \psi^*$  are extended to  $\Omega$  using the Bloch periodicity condition, i.e.,

$$\psi(\theta, x) = e^{i\theta s} \psi_0(\theta, x), \quad \psi^*(\theta, x) = e^{i\theta s} \psi_0^*(\theta, x), \quad (17)$$

where the functions  $\psi_0, \psi_0^*$  are periodic with respect to  $s$ . The second term in (16) can be estimated similarly to  $u_2$ . Thus

$$u(t, x) = \frac{1}{2\pi} \int_{|\theta| < \delta} \int_{\Omega'} \psi(\theta, x) \overline{\psi^*}(\theta, y) e^{\lambda_0(\theta)t} \widehat{\varphi} dy d\theta + w(t, x),$$

where  $x \in \Omega$ ,  $t > 1$ , and

$$|w| \leq \frac{C}{\sqrt{\varepsilon}} e^{-\gamma t} \|\varphi(x)\|_{L_2(\mathbb{R}^d)} = O(\varepsilon) \quad \text{if } t > \frac{t_0}{\varepsilon^2}, \quad \varphi \in L_{1, \text{com}}. \quad (18)$$

Let  $y = (s', z')$ . Then

$$\widehat{\varphi} = \sum_{n=-\infty}^{\infty} \varphi(\varepsilon(s' - n), z') e^{in\theta}.$$

Hence (with (17) taken into account), we have

$$\begin{aligned}
u(t, x) &= \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \int_{|\theta| < \delta} \int_{\Omega'} e^{i\theta(s-s'+n)} \psi_0(\theta, x) \overline{\psi_0^*}(\theta, y) e^{\lambda_0(\theta)t} \varphi(\varepsilon(s' - n), z') dy d\theta + O(\varepsilon) \\
&= \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \int_{|\theta| < \delta} \int_{\Omega(n)} e^{i\theta(s-s')} \psi_0(\theta, x) \overline{\psi_0^*}(\theta, y) e^{\lambda_0(\theta)t} \varphi(\varepsilon s', z') dy d\theta + O(\varepsilon) \\
&= \frac{1}{2\pi} \int_{|\theta| < \delta} \int_{\Omega} e^{i\theta(s-s')} \psi_0(\theta, x) \overline{\psi_0^*}(\theta, y) e^{\lambda_0(\theta)t} \varphi(\varepsilon s', z') dy d\theta + O(\varepsilon). \quad (19)
\end{aligned}$$

We split the double integral  $I$  above in two parts  $I = I_1 + I_2$ , where the integration in  $\theta$  in the part  $I_1$  extends only over the segment  $|\theta^3 t| < 1$ ,  $t \geq \delta^{-3}$ , and  $I_2 = I - I_1$ . From Lemma 2.2 it follows that  $\operatorname{Re} \lambda_0(\theta) < -\frac{\sigma^2}{2} \theta^2$ ,  $|\theta| < \delta$ , if  $\delta$  is small enough. Since we can take  $\delta$  as small as we please, and the functions  $\psi_0, \psi_0^*$  are bounded, it follows that

$$I_2 \leq C \int_{|\theta| > t^{-1/3}} \int_{\Omega} e^{-\frac{\sigma^2}{2} \theta^2 t} |\varphi(\varepsilon s', z')| dy d\theta = \frac{\|\varphi(x)\|_{L_1(\mathbb{R}^d)}}{\varepsilon} O(e^{-\frac{\sigma^2}{2} t^{1/3}}) = O(\varepsilon), \quad t > \frac{\tau_0}{\varepsilon^2}.$$

We replace  $\lambda_0(\theta)$  in the integral  $I_1$  by its quadratic approximation found in Lemma 2.2:

$$e^{\lambda_0(\theta)t} = e^{(iV_{\text{eff}}\theta - \sigma^2 \theta^2)t} (1 + O(|\theta|^3 t)).$$

If only the remainder term is taken into account, then the corresponding integral can be estimated by

$$\begin{aligned}
C \int_{|\theta| < t^{-1/3}} \int_{\Omega} |\theta|^3 t e^{-\sigma^2 \theta^2 t} \varphi(\varepsilon s', z') dy d\theta &\leq \frac{C}{\varepsilon} \|\varphi(y)\|_{L_1(\mathbb{R}^d)} \int_{-\infty}^{\infty} |\theta|^3 t e^{-\sigma^2 \theta^2 t} d\theta \\
&= \frac{C}{t\varepsilon} \|\varphi(y)\|_{L_1(\mathbb{R}^d)} = O(\varepsilon), \quad \text{if } t > \frac{\tau_0}{\varepsilon^2}.
\end{aligned}$$

From here and (19) it follows that

$$u(t, x) = \frac{1}{2\pi} \int_{|\theta| < t^{-1/3}} \int_{\Omega} e^{i\theta(s-s')} \psi_0(\theta, x) \overline{\psi_0^*}(\theta, y) e^{(iV_{\text{eff}}\theta - \sigma^2 \theta^2)t} \varphi(\varepsilon s', z') dy d\theta + O(\varepsilon), \quad t > \frac{\tau_0}{\varepsilon^2}.$$

We put  $\theta = 0$  in the arguments of functions  $\psi_0$  and  $\overline{\psi_0^*}$ . Since these functions are periodic,  $\psi_0 = 1$  and  $\psi_0^*(0, y) = \pi(y)$  is real, we obtain that  $\psi_0(\theta, x) \overline{\psi_0^*}(\theta, y) = \pi(y) + O(|\theta|)$ . We put this relation into the formula above and note that the integral with the term  $O(|\theta|)$  does not exceed

$$\begin{aligned}
C \int_{|\theta| < t^{-1/3}} \int_{\Omega} |\theta| e^{-\sigma^2 \theta^2 t} \varphi(\varepsilon s', z') dy d\theta &\leq \frac{C}{\varepsilon} \|\varphi(y)\|_{L_1(\mathbb{R}^d)} \int_{-\infty}^{\infty} |\theta| e^{-\sigma^2 \theta^2 t} d\theta \\
&= \frac{C}{t\varepsilon} \|\varphi(y)\|_{L_1(\mathbb{R}^d)} = O(\varepsilon), \quad \text{if } t > \frac{\tau_0}{\varepsilon^2}.
\end{aligned}$$

Hence if  $t > \tau_0/\varepsilon^2$ , then

$$u(t, x) = \frac{1}{2\pi} \int_{|\theta| < t^{-1/3}} \int_{\Omega} e^{i\theta(s-s')} \pi(y) e^{(iV_{\text{eff}}\theta - \sigma^2\theta^2)t} \varphi(\varepsilon s', z') dy d\theta + O(\varepsilon), \quad y = (s', z').$$

We can replace here the integration in  $\theta$  over the interval  $|\theta| < t^{-1/3}$  by the integration over the whole line since the difference between the corresponding integrals decays exponentially as  $t \rightarrow \infty$ . Thus

$$u(t, x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{\Omega} e^{i\theta(s-s')} \pi(y) e^{(iV_{\text{eff}}\theta - \sigma^2\theta^2)t} \varphi(\varepsilon s', z') dy d\theta + O(\varepsilon), \quad t > \tau_0/\varepsilon^2.$$

The integral  $w = w(t, s)$  above does not depend on  $z$ . By simple differentiation one can check that the integral satisfies equation (2). Function  $w(0, s)$  is the Fourier transform in  $s'$  followed by its inverse (in  $\theta$ ), i.e.,

$$w(0, s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{S_{s'}} e^{i\theta(s-s')} \pi(s', z') \varphi(\varepsilon s', z') dz' ds' d\theta = \int_{S_s} \pi(s, z') \varphi(\varepsilon s, z') dz', \quad (20)$$

where  $S_a$  is the cross-section of  $\Omega$  by the plane through  $s = a$ . Thus  $w$  is the solution of problem (2) with  $w_0$  given in (5), and the first statement of Theorem 2.1 is proved.

In order to prove the second statement of Theorem 2.1, we will show that  $w - \bar{w} = O(\varepsilon)$ ,  $\tau > \tau_0$ . We denote function  $w$  in new coordinates by  $\hat{w}$ , i.e.,  $\hat{w}(\tau, \varsigma) = w(\frac{\tau}{\varepsilon^2}, \frac{\varsigma - V_{\text{eff}}\tau}{\varepsilon})$ . Obviously,  $\hat{w}$  satisfies the same equation as the equation for  $\bar{w}$ , and  $\hat{w}(0, \varsigma) = w_0(\frac{\varsigma}{\varepsilon}, \varsigma)$ . The solution of the initial problem for  $\hat{w}$  is the convolution of the smooth (when  $\tau > \tau_0$ ) kernel  $K = \frac{1}{\sqrt{4\pi\sigma\tau}} e^{-\frac{\varsigma^2}{4\sigma\tau}}$  and  $w_0(\frac{\varsigma}{\varepsilon}, \varsigma)$ . The second factor is periodic in the first argument (see (5)). Thus, the convolution differs by  $O(\varepsilon)$  from the same convolution when the second factor is replaced by its average with respect to the first argument. This second convolution is  $\bar{w}$ . This completes the proof of the second statement of the Theorem 2.1.

It remains to note that in the proof of Theorem 2.1 it was shown that the effective drift and the effective diffusivity were defined by the coefficients of the Taylor expansion of the eigenvalue  $\lambda_0(\theta)$ . Thus, Theorem 2.3 was also established.  $\square$

In conclusion of this section we will provide some formulas that can be useful for practical evaluation of the effective drift  $V_{\text{eff}}$  and the effective diffusivity  $\sigma^2$ .

Let

$$v = 1 + i\theta v_1(x) - \theta^2 v_2(x) + O(\theta^3), \quad \theta \rightarrow 0, \quad (21)$$

be the Taylor expansion at zero of the principal eigenfunction of the problem (3) with the eigenvalue  $\lambda = \lambda_0(\theta)$ . We plug (21) and the expansion for  $\lambda_0(\theta)$  from Lemma 2.2 into (3) and take into account that conditions on  $S_0, S_1$  in (3) can be rewritten as the periodicity in  $s = x_1$  of the function  $e^{ix\theta}v$ . Then we obtain the following problems for the coefficients  $v_1, v_2$ :

$$\Delta v_1 + V \frac{\partial v_1}{\partial s} = V_{\text{eff}}, \quad x \in \Omega'; \quad \frac{\partial v_1}{\partial n}|_{S^i} = 0; \quad v_1 = s + \psi_1(x), \quad (22)$$

$$\Delta v_2 + V \frac{\partial v_2}{\partial s} = V_{\text{eff}} v_1 + \sigma^2, \quad x \in \Omega'; \quad \frac{\partial v_2}{\partial n}|_{S^l} = 0; \quad v_2 = \frac{s^2}{2} + s\psi_1(x) + \psi_2(x), \quad (23)$$

where the functions  $\psi_1, \psi_2$  are periodic. Function  $v_1$  is called the *harmonic coordinate*. Usually the harmonic coordinate satisfies a homogeneous equation, but this equation (see (22)) becomes inhomogeneous in the presence of a drift in the problem. Denote by  $\pi = \pi(x)$  the principal eigenfunction with eigenvalue  $\lambda = 0$  for the adjoint problem (4) with  $\theta = 0$ , i.e.,

$$\Delta \pi - V \frac{\partial \pi}{\partial s} = 0, \quad x \in \Omega'; \quad \left( \frac{\partial}{\partial n} - V n_1 \right) \pi|_{S^l} = 0; \quad \pi|_{S_1} = \pi|_{S_0}, \quad \pi'_s|_{S_1} = \pi'_s|_{S_0}. \quad (24)$$

This is a positive function due to the Perron-Frobenius theorem (see details in the proof of Lemma 2.5). We normalize  $\pi$  by the condition  $\int_{\Omega'} \pi dx = 1$ . This function is *the density of the invariant measure*. Note that  $\pi(x) \equiv 1/|\Omega'|$  if  $V = 0$ .

**Theorem 2.5.** *The effective drift  $V_{\text{eff}}$  can be found from either of the following three formulas:*

$$V_{\text{eff}} = \int_S (V\pi - \pi'_s) dS = V - \int_{\Omega'} \pi'_s dx = V - \int_{\partial S^l} n_1 \pi dS, \quad (25)$$

where  $S$  is a cross-section of the domain  $\Omega$  by an arbitrary hyperplane  $s = \text{const.}$ ,  $n_1$  is the first component of the outward normal vector  $n$ , and  $S^l = \partial\Omega' \setminus [S_0 \cup S_1]$  is the lateral part of the boundary of  $\Omega'$ . The effective diffusivity is given by

$$\sigma^2 = \int_{\Omega'} |\nabla v_1|^2 \pi dx. \quad (26)$$

**Remark.** If  $V = 0$ , then formula (26) is equivalent to the following one

$$\sigma^2 = 1 - \frac{\int_{\Omega'} |\nabla \psi_1|^2 dx}{|\Omega'|}.$$

The latter formula shows that the effective diffusivity is always smaller than in the free space if  $\Omega$  is not a cylinder (i.e., if  $\psi_1$  is not identical zero).

**Proof.** The remark will be justified at the end of the proof of the theorem. Let  $L = \Delta + V \frac{\partial}{\partial s}$  be the differential expression in the left-hand side of (22), and let  $L^* = \Delta - V \frac{\partial}{\partial s}$  be the conjugate expression (see (24)). Since  $L^* \pi = 0$  and  $v_1$  satisfies (22), we have

$$\int_{\Omega'} (Lv_1) \pi dx - \int_{\Omega'} v_1 L^* \pi dx = V_{\text{eff}} \int_{\Omega'} \pi dx = V_{\text{eff}}.$$

The left-hand side here can be rewritten using the Green's formula and the divergence theorem applied to the vector field  $\vec{F} = (v_1 \pi, 0, 0)$ . This leads to

$$V_{\text{eff}} \int_{\Omega'} \pi dx = \int_{\partial\Omega'} \left[ (\Delta v_1) \pi - v_1 \Delta \pi + V \frac{\partial(v_1 \pi)}{\partial s} \right] dx = \int_{\partial\Omega'} \left( \frac{\partial v_1}{\partial n} \pi - v_1 \frac{\partial \pi}{\partial n} + V v_1 \pi n_1 \right) dS.$$

The second integrand vanishes on  $S^l$  since  $\pi$  satisfies the boundary condition (24) on  $S^l$  and  $\frac{\partial v_1}{\partial n} = 0$  on  $S^l$ . Thus

$$V_{\text{eff}} \int_{\Omega'} \pi dx = \int_{S_0 \cup S_1} \left( \frac{\partial v_1}{\partial n} \pi - v_1 \frac{\partial \pi}{\partial n} + V v_1 \pi n_1 \right) dS. \quad (27)$$

We substitute here  $v_1 = s + \psi_1$ . The integral with  $\psi_1$  is zero due to the periodicity of the functions  $\psi_1$  and  $\pi$ . Thus (27) holds with  $v_1$  replaced by  $s$ . If we also take into account that

$$\int_{S_0 \cup S_1} \frac{\partial s}{\partial n} \pi dS = 0,$$

then we obtain the first equality (25) with  $S = S_1$ . Then this equality holds with any  $S$  since  $V_{\text{eff}}$  is invariant with respect to the shift  $s \rightarrow s + a$ . Let us provide another way to show that the middle term in (25) does not depend on the choice of  $S$ . Let  $\Omega_{a,b} = \Omega \cap \{a < s < b\}$ . Then

$$\begin{aligned} 0 &= \int_{\Omega_{a,b}} L^* \pi dx = \int_{\partial \Omega_{a,b}} (\pi'_n - V \pi n_1) dS = \int_{S_a \cup S_b} (\pi'_n - V \pi n_1) dS \\ &= \int_{S_b} (\pi'_s - V \pi) dS - \int_{S_a} (\pi'_s - V \pi) dS. \end{aligned}$$

In order to prove the second equality (25), we write the first one with  $S = S_a$  and integrate with respect to  $a$  over the interval  $(0, 1)$ . The last equality (25) follows from the divergence theorem.

The proof of (26) is similar. We have

$$\int_{\Omega'} (V_{\text{eff}} v_1 + \sigma^2) \pi dx = \int_{\Omega'} (L v_2) \pi dx - \int_{\Omega'} v_2 L^* \pi dx = \int_{S_0 \cup S_1} \left( \frac{\partial v_2}{\partial n} \pi - v_2 \frac{\partial \pi}{\partial n} + V v_2 \pi n_1 \right) dS.$$

We plug here  $v_2 = \frac{s^2}{2} + s\psi_1 + \psi_2$ . The integral with  $\psi_2$  vanishes due to the periodicity of  $\psi_2$  and  $\pi$ . Hence  $v_2$  can be replaced by  $\frac{s^2}{2} + s\psi_1$ . We reduce the integral over  $S_0$  to an integral over  $S_1$  using the substitution  $s \rightarrow s - 1$ . Taking into account the periodicity of  $\psi_1$  and  $\pi$  we obtain

$$\begin{aligned} \int_{\Omega'} (V_{\text{eff}} v_1 + \sigma^2) \pi dx &= \int_{S_1} \left[ \left(1 + \frac{\partial \psi_1}{\partial s}\right) \pi - \left(\frac{1}{2} + \psi_1\right) \frac{\partial \pi}{\partial s} + V \left(\frac{1}{2} + \psi_1\right) \pi \right] dS \\ &= \int_{S_1} \left[ \frac{\partial v_1}{\partial s} \pi - v_1 \frac{\partial \pi}{\partial s} + V v_1 \pi \right] dS - \frac{1}{2} V_{\text{eff}}. \end{aligned}$$

The last relation is the consequence of the first equality (25) and the equality  $v_1 = s + \psi_1$ . Hence,

$$\sigma^2 = \int_{S_0} \left[ \frac{\partial v_1}{\partial s} \pi - v_1 \frac{\partial \pi}{\partial s} + V v_1 \pi \right] dS - V_{\text{eff}} \int_{\Omega'} v_1 \pi dx - \frac{1}{2} V_{\text{eff}}. \quad (28)$$

It remains to show that

$$\int_{\Omega'} |\nabla v_1|^2 \pi dx = \int_{S_0} \left[ \frac{\partial v_1}{\partial s} \pi - v_1 \frac{\partial \pi}{\partial s} + V v_1 \pi \right] dS - V_{\text{eff}} \int_{\Omega'} v_1 \pi dx - \frac{1}{2} V_{\text{eff}}. \quad (29)$$

We note that  $L(v_1^2) = 2v_1 L v_1 + 2|\nabla v_1|^2 = 2V_{\text{eff}} v_1 + 2|\nabla v_1|^2$ . Thus

$$\begin{aligned} \int_{\Omega'} |\nabla v_1|^2 \pi dx &= \frac{1}{2} \int_{\Omega'} L(v_1^2) \pi dx - V_{\text{eff}} \int_{\Omega'} v_1 \pi dx \\ &= \int_{S_0 \cup S_1} \left[ v_1 \frac{\partial v_1}{\partial n} \pi - \frac{1}{2} v_1^2 \left( \frac{\partial \pi}{\partial n} - V \pi n_1 \right) \right] dS - V_{\text{eff}} \int_{\Omega'} v_1 \pi dx. \end{aligned}$$

We took into account here that the integrand of the first term on the right vanishes at  $S^l$ . The last inequality implies (29) if the integral over  $S_1$  in the equality above is rewritten in terms of the integral over  $S_0$  using the first formula (25) and periodicity of the functions  $\pi$  and  $v_1 - s$ . The proof of the theorem is complete. Now let us justify the remark.

From the divergence theorem and periodicity of  $\psi_1$  it follows that

$$\int_{\Omega'} \frac{\partial \psi_1}{\partial s} dx = \int_{\partial \Omega'} \psi_1 n_1 dS = \int_{S^l} \psi_1 n_1 dS.$$

Since  $n_1 = \frac{\partial s}{\partial n}$  and the latter function on  $S^l$  is equal to  $-\frac{\partial \psi_1}{\partial n}$  (due to (22)), we have

$$\int_{\Omega'} \frac{\partial \psi_1}{\partial s} dx = \int_{\partial \Omega'} \psi_1 n_1 dS = - \int_{S^l} \psi_1 \frac{\partial \psi_1}{\partial n} dS = - \int_{\partial \Omega'} \psi_1 \frac{\partial \psi_1}{\partial n} dS.$$

Now we recall that  $\Delta \psi_1 = \Delta(v_1 - s) = 0$ . Hence the latter formula together with the Green formula imply

$$\int_{\Omega'} \frac{\partial \psi_1}{\partial s} dx = - \int_{\Omega'} |\nabla \psi_1|^2 dx. \quad (30)$$

Further, if  $V = 0$ , then  $\pi = 1/|\Omega'|$ . From  $v_1 = \psi_1 + s$ , (26) and (30) it follows that

$$\sigma^2 |\Omega'| = \int_{\Omega'} |\nabla v_1|^2 dx = \int_{\Omega'} \left( 1 + 2 \frac{\partial \psi_1}{\partial s} + |\nabla \psi_1|^2 \right) dx = \int_{\Omega'} (1 - |\nabla \psi_1|^2) dx$$

□

**Theorem 2.6.** *If  $V = 0$  then  $V_{\text{eff}} = 0$ , and  $V_{\text{eff}} = \sigma_0^2 V + O(V^2)$  as  $V \rightarrow 0$  where  $\sigma_0^2 = \sigma^2|_{V=0} > 0$  is the effective diffusivity at  $V = 0$ . In particular, if  $|V|$  is small enough, then  $V_{\text{eff}} \neq 0$  when  $V \neq 0$  and  $V_{\text{eff}}$  is a monotone function of  $V$ .*

**Proof.** From (24) it follows that  $\pi$  is an analytic function of  $V$ . Then (25) implies that  $V_{\text{eff}}$  is analytic in  $V$ , and (22) implies that  $v_1$  and  $\psi_1$  depend on  $V$  analytically. We extend  $\pi = \frac{1}{|\Omega'|} + V \pi_1 + O(V^2)$  in the Taylor series at  $V = 0$ . Then (24) leads to the following problem for  $\pi_1$ :

$$\Delta \pi_1 = 0, \quad x \in \Omega'; \quad \frac{\partial \pi_1}{\partial n} \Big|_{S^l} = \frac{n_1}{|\Omega'|}; \quad \pi_1|_{S_1} = \pi_1|_{S_0}, \quad (\pi_1)'_s|_{S_1} = (\pi_1)'_s|_{S_0}.$$



Since  $n_1 = \frac{\partial s}{\partial n}$ , only the factor  $-1/|\Omega'|$  in the boundary condition makes the problem for  $\pi_1$  different from the problem for  $\psi_1^0 = \psi_1|_{V=0}$ . The latter problem can be obtained from (22) if we put there  $V = V_{\text{eff}} = 0$ . Hence  $\pi_1 = -\frac{\psi_1^0}{|\Omega'|}$ , i.e.,  $\pi = \frac{1}{|\Omega'|} - \frac{V\psi_1^0}{|\Omega'|} + O(V^2)$ . We put this into the second of relations (25) and obtain that

$$V_{\text{eff}} = V(1 + \frac{\int_{\Omega'} (\psi_1^0)'_s dx}{|\Omega'|}) + O(V^2) = V(1 - \frac{\int_{\Omega'} |\nabla \psi_1^0|^2 dx}{|\Omega'|}) + O(V^2).$$

The last relation follows from (30). It remains only to use the Remark after Theorem 2.5.  $\square$

### 3 Periodic tubes with nearly separated dead zones.

Consider the problem (1) with  $V = 0$  (without drift) in a periodic domain  $\Omega = \Omega(\varepsilon) \subset \mathbb{R}^d$  introduced in the previous section, that has the form of an  $\varepsilon$ -independent periodic tube  $\Omega_0$  with a periodic system of cavities connected to the tube  $\Omega_0$  by narrow channels (see Fig. 3). In this section we'll assume that  $d \geq 3$ . We do not impose restrictions on the shape of channels, except the periodicity condition, smoothness of the boundary  $\partial\Omega(\varepsilon)$  and the assumption that the channel enters the cell of periodicity  $\Omega'_0$  of the main tube in an  $\varepsilon$  neighborhood of some point  $x_0 \in \partial\Omega'_0$ . For simplicity we will assume that there is only one cavity and one channel on each period, but practically no changes are needed to extend all the arguments to the case of several cavities per period or multiple channels connecting the cavity with the tube.

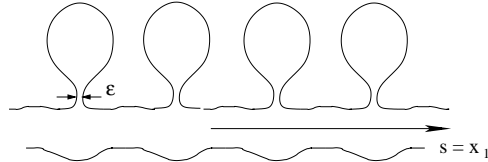


Figure 3: Periodic tube with nearly separated cavities (dead zones).

Denote by  $\Omega'(\varepsilon) = \Omega'_0 \cup \Omega'_1(\varepsilon)$  one cell of periodicity of the domain  $\Omega(\varepsilon)$ , where  $\Omega'_0$  is the cell of periodicity of the main tube  $\Omega_0$  and  $\Omega'_1(\varepsilon)$  is the union of the cavity and the channel on this period. We assume that the cell  $\Omega'_0$  is defined by the restriction  $0 < s = x_1 < 1$ . We denote by  $S_0, S_1$  the parts of the boundary of  $\Omega'_0$  that belong to the planes through the points  $s = 0$  and  $s = 1$ , respectively. Let  $S^l = \partial\Omega'_0 \setminus [S_0 \cup S_1]$  be the lateral part of the boundary  $\partial\Omega'_0$  of the cell of the main tube.

In order to describe the effective diffusivity  $\sigma^2$  for the problem in  $\Omega(\varepsilon)$  and the effective diffusivity  $\sigma_0^2$  for the problem in the main tube  $\Omega_0$  (without the cavities and channels), we introduce the following auxiliary problem

$$\Delta u = 0, \quad x \in \Omega_0; \quad u = s + \psi, \quad \text{where } \psi \text{ is 1-periodic in } s; \quad u'_n|_{S^l} = 0. \quad (31)$$

We will call function  $u$  the harmonic coordinate (for the domain  $\Omega_0$ ). This function was introduced in the previous section where it was denoted by  $v_1$  (see (22)).

**Theorem 3.1.** *Let  $V = 0$ . Then the following formulas are valid for the effective diffusivity  $\sigma_0^2$  in the case of a periodic tube  $\Omega_0$  and for the effective diffusivity  $\sigma_0^2(\varepsilon)$  in the case of the tube  $\Omega_0$  with cavities:*

$$\sigma_0^2 = \frac{\int_{\Omega'_0} |\nabla u|^2 dx}{|\Omega'_0|}, \quad (32)$$

$$\sigma^2(\varepsilon) = \frac{|\Omega'_0| \sigma_0^2}{|\Omega'_0| + |\Omega'_1(\varepsilon)|} + O(\varepsilon^{d-2}), \quad \varepsilon \rightarrow 0. \quad (33)$$

**Remark.** When  $\Omega_0$  is a cylinder, formula (33) under some assumptions on the connecting channels can be found in [1], [4].

**Proof.** In the case of domain  $\Omega_0$ , we will use notations  $u, \psi$  for functions  $v_1, \psi_1$ , defined in (21), (22) (compare (22) and (31)), and we preserve the original notations  $v_1, \psi_1$  when the problem in  $\Omega(\varepsilon)$  is considered.

We note that  $\pi$  is a constant when  $V = 0$ . From the normalization condition ( $\int_{\Omega'} \pi dx = 1$ ) it follows that  $\pi = 1/|\Omega'_0|$  for the problem in  $\Omega_0$  and  $\pi = 1/|\Omega'_0(\varepsilon)|$  for the problem in  $\Omega_0(\varepsilon)$ . Hence, formula (32) follows from (26). In fact, (26) was derived without any specific assumptions on the periodic domain  $\Omega$ , and it is valid for both domains  $\Omega_0$  and  $\Omega(\varepsilon)$ . Thus

$$\sigma^2(\varepsilon) = \frac{\int_{\Omega'(\varepsilon)} |\nabla v_1|^2 dx}{|\Omega'(\varepsilon)|}. \quad (34)$$

We are going to compare the functions  $u$  and  $v_1$  and derive (33) from (34) and (32).

Let  $x_0 \in S^l$  be the point on the lateral side of the cell  $\Omega'_0$  where the channel enters the main tube. Harmonic coordinates  $u$  and  $v_1$  (for tubes  $\Omega_0$  and  $\Omega(\varepsilon)$ , respectively) are defined up to arbitrary additive constants. We fix these constants assuming that  $u(x_0) = v_1(x_0) = 0$ .

We fix a function  $\alpha = \alpha(\varepsilon, x) \in C^\infty(\Omega'_0)$  such that  $\alpha = 0$  when  $|x - x_0| < 2\varepsilon$ ,  $\alpha = 1$  when  $|x - x_0| > 3\varepsilon$  and  $\frac{\partial \alpha}{\partial n} = 0$  on  $S^l$ . We consider function  $w = \alpha(x)u(x)$  and extend it by zero in the channel and the cavity. Then  $w \in C^\infty(\Omega'(\varepsilon))$ .

Let us estimate  $v_1 - w$ . Obviously, this difference satisfies the following relations in  $\Omega(\varepsilon)$ :

$$\Delta(v_1 - w) = f := 2\nabla \alpha \nabla u + u \Delta \alpha, \quad x \in \Omega(\varepsilon); \quad \frac{\partial(v_1 - w)}{\partial n} = 0, \quad x \in S^l(\varepsilon), \quad (35)$$

and it satisfies the periodicity condition on  $S_0, S_1$ . Function  $u$  is smooth and  $\varepsilon$ -independent. Function  $\nabla \alpha$  has order  $O(\varepsilon^{-1})$ , and its support belongs to a ball of radius  $3\varepsilon$ . Thus  $\|\nabla \alpha \nabla u\|_{L_2(\Omega'(\varepsilon))} = O(\varepsilon^{\frac{d-2}{2}})$ ,  $\varepsilon \rightarrow 0$ . A similar estimate is valid for  $u \Delta \alpha$  since  $\Delta \alpha = O(\varepsilon^{-2})$  and  $|u| < C\varepsilon$  on the support of  $\Delta \alpha$ . Hence  $\|f\|_{L_2(\Omega'(\varepsilon))} = O(\varepsilon^{\frac{d-2}{2}})$ ,  $\varepsilon \rightarrow 0$ . We

also take into account that the support of  $f$  belongs to  $\Omega'_0$ . Thus from the Green formula it follows that

$$\|\nabla(v_1 - w)\|_{L_2(\Omega'(\varepsilon))}^2 \leq C\|f\|_{L_2(\Omega'(\varepsilon))}\|v_1 - w\|_{L_2(\Omega'_0)} = O(\varepsilon^{\frac{d-2}{2}})\|v_1 - w\|_{L_2(\Omega'_0)}, \quad \varepsilon \rightarrow 0. \quad (36)$$

Since domain  $\Omega'_0$  does not depend on  $\varepsilon$  and  $(v_1 - w)(x_0) = 0$ , we have  $\|v_1 - w\|_{L_2(\Omega'_0)} \leq C\|\nabla(v_1 - w)\|_{L_2(\Omega'_0)}$ . Hence from (36) it follows that

$$\|\nabla(v_1 - w)\|_{L_2(\Omega'(\varepsilon))} = O(\varepsilon^{\frac{d-2}{2}}). \quad \varepsilon \rightarrow 0. \quad (37)$$

Thus one can make the following changes in formula (34) with the accuracy of  $O(\varepsilon^{d-2})$ : replace  $v_1$  by  $\alpha u$ , replace integration over  $\Omega'(\varepsilon)$  by the integration over  $\Omega'_0$ , and then drop  $\alpha$ . In other words, one can replace the numerator in (34) by the numerator from (32) plus  $O(\varepsilon^{d-2})$ . Then it remains only to use (32) and express the latter numerator through  $\sigma_0^2$ .  $\square$

## References

- [1] A. Berezhkovskii, L. Dagdug, Analytic treatment of biased diffusion in tubes with periodic dead ends, J. Chemical Phys., 134 (2011), 124109.
- [2] C. Conca, M. Vanninathan, Homogenization of periodic structures via Bloch decomposition, Siam J. Appl. Math. 57, No. 6 (1997) pp. 1639-1659.
- [3] C. Conca, R. Orive, M. Vanninathan, Bloch approximation in homogenization on bounded domains, Asymptot. Anal. 41 (2005), No. 1, 71-91.
- [4] L. Dagdug, A. Berezhkovskii, Y. Makhnovskii, V. Zitserman, Transient diffusion in the tube with dead ends, J. Chemical Phys., 127 (2007), 224712.
- [5] G. Grubb, Functional Calculus of Pseudodifferential Boundary Problems, Birkhauser, Boston, 1996.
- [6] P. Reimann, Brownian motors: noisy transport far from equilibrium, Physical reports, 361 (2002), 57-265.